Nuclear Instruments and Methods in Physics Research B 102 (1995) xiii–xv

ELSEVIER

NIM B
Beam Interactions with Materials & Atoms

Contents

Preface vii
Advisors, committees and sponsors viii
Photos ix

Section I. Interatomic potentials and theoretical methods

A multisite interaction expansion of the total energy in metals
E.C. Sowa and A. Gonis 1
Comparison of channeling trajectories and ranges calculated by the continuum potential approximation and Crystal-TRIM
Q.K.K. Liu, J.P. Biersack and M. Posselt 3
An improved molecular dynamics scheme for ion bombardment simulations
L.A. Marqués, J.E. Rubio, M. Jaraíz, L. Enríquez and J. Barbolla 7
The influence of impurity trapping on formation and growth of defect clusters in irradiated materials
Y. Katoh and A. Kohyama 12
Relocation cross-sections in silicon: theoretical models
M.J. Caturla, V. Konoplev, I. Abril and A. Gras-Marti 19
Acceleration of binary collision simulations in crystalline targets using critical angles for ion channeling
G. Hobler and A. Simionescu 24
Ab initio pseudopotential calculations of point defects and boron impurity in silicon
Jing Zhu, L.H. Yang, C. Mailhiot, T. Diaz de la Rubia and G.H. Gilmer 29
Escape probabilities for electrons emitted during the interaction of slow highly charged ions with metal surfaces
C. Lemell, HP. Winter, F. Aumayr, J. Burgdörfer and C. Reinhold 33

Section II. Displacement cascades and radiation effects in metals

Computer simulation of defect production by displacement cascades in metals
D.J. Bacon, A.F. Calder, F. Gao, V.G. Kapinos and S.J. Wooding 37
Simulating the production of free defects in irradiated metals
H.L. Heinisch 47
Surface effects on damage production during ion bombardment: a molecular dynamics study
M. Ghaly, R.S. Averback and T. Diaz de la Rubia 51
Molecular Dynamics Simulations of displacement cascades in metallic systems
N.V. Doan and H. Tietze 58
The correlation of defect distribution in collisional phase with measured cascade collapse probability
K. Morishita, H.L. Heinisch, S. Ishino and N. Sekimura 67
Phase evolution under irradiation: Monte Carlo and mean-field modelings
P. Bellon, Y. Grandjean, M. Przybylowicz, F. Soisson and G. Martin 72
Collision cascades in Zr_2Fe, Zr_3Fe and $ZrFe_2$
L.M. Howe, D. Phillips, H.H. Plattner and J.D. Bonnett 77
Computer simulations of disordering and amorphization kinetics in intermetallic compounds
M. Spaczér, A. Caro, M. Victoria and T. Diaz de la Rubia 81
Momentum in atomic collision cascades
M.W. Sckerl, M. Vicanek and P. Sigmund 86

0168-583X/95/$09.50 © 1995 Elsevier Science B.V. All rights reserved

Cascade statistics in the binary collision approximation and in full molecular dynamics
M. Hou and Z-Y. Pan 93
Radiation cleansing of vacancies
R.A. Johnson 103
Simulation of plastic deformation of small iron and copper single crystals
M. Doyama 107
The effect of neutron energy on defect production in alumina
M.B. Lee and E.H. Farnum 113
Simulation of radiation induced structural transformation in glassy metals
T. Mattila, R.M. Nieminen and M. Dzugutov 119
Impact of glissile interstitial loop production in cascades on void ordering and swelling saturation under irradiation
V.I. Dubinko 125
Increasing the retained dose by plasma immersion ion implantation and . deposition
A. Anders, S. Anders, I.G. Brown and K.M. Yu 132
Dynamic Monte Carlo simulation for ion beam mixing
H.J. Kang, S.C. Lee, S.M. Jung, I.S. Choi and C.N. Whang 136
CASSIS – a new Monte-Carlo computer program for channeling simulation of RBS, NRA and PIXE
A. Kling 141
An investigation of collision propagation in energetic ion initiated cascades in copper
I.R. Chakarov, R.P. Webb, R. Smith and K. Beardmore 145
Numerical analysis of stress effects on Frank loop evolution during irradiation in austenitic Fe–Cr–Ni alloy
H. Tanigawa, Y. Katoh and A. Kohyama 151
A new model of vacancy loop nucleation in irradiated metals
V.G. Kapinos and D.J. Bacon 156

Section III. Radiation effects in semiconductors

Challenges for predictive process simulation in sub 0.1 μm silicon devices
J.D. Plummer and P.B. Griffin 160
Dynamic simulation of damage accumulation during implantation of BF_2^+ molecular ions into crystalline silicon
M. Posselt 167
Modeling of ion implantation in single-crystal silicon
A.F. Tasch, S.-H. Yang and S.J. Morris 173
Defects from implantation in silicon by linked Marlowe–molecular dynamics calculations
M. Jaraiz, G.H. Gilmer, D.M. Stock and T. Diaz de la Rubia 180
Round robin computer simulation of ion transmission through crystalline layers
K. Gärtner, D. Stock, B. Weber, G. Betz, M. Hautala, G. Hobler, M. Hou, S. Sarite, W. Eckstein, J.J. Jiménez-Rodríguez, A.M.C. Pérez-Martín, E.P. Andribet, V. Konoplev, A. Gras-Marti, M. Posselt, M.H. Shapiro, T.A. Tombrello, H.M. Urbassek, H. Hensel, Y. Yamamura and W. Takeuchi 183
Process simulation challenges for ULSI devices: a users perspective
M.I. Current, R. Mathur, M. Kump and L.A. Larson 198
Modelling of amorphous zones in semiconductors by using the randomization-and-relaxation method
I. Jenčič, J. Peternelj and I.M. Robertson 202
Point defect accumulation in silicon irradiated by energetic particles: A molecular dynamics simulation
D.M. Stock, G.H. Gilmer, M. Jaraíz and T. Diaz de la Rubia 207
A molecular dynamics study of energetic particle impacts on carbon and silicon
R. Smith, K. Beardmore, A. Gras-Marti, R. Kirchner and R.P. Webb 211
Molecular dynamics simulations of implantation damage and recovery in semiconductors
M. Sayed, J.H. Jefferson, A.B. Walker and A.G. Cullis 218

Ion bombardment of polyethylene
K. Beardmore and R. Smith 223
Low energy ion implantation simulation using a modified binary collision approximation code
J. Arias, M. Jaraiz, L. Pelaz, L.A. Bailón and J. Barbolla 228
Computer simulation of atomic displacements in Si, GaAs, and AlAs
M. Sayed, J.H. Jefferson, A.B. Walker and A.G. Cullis 232
Comparison of BC and MD simulations of low-energy ion implantation
M. Posselt and K.-H. Heinig 236
Improved efficiency in Monte Carlo simulation of ion implanted impurity profiles in single-crystal materials
S.-H. Yang, D. Lim, S.J. Morris and A.F. Tasch 242
Diffusion and interactions of point defects in silicon: molecular dynamics simulations
G.H. Gilmer, T. Diaz de la Rubia, D.M. Stock and M. Jaraiz 247
Computer simulation of mechanisms of the SIMOX process
S. Reiss and K.-H. Heinig 256

Section IV. Sputtering and surface processes

Preferential sputtering of alloys: a molecular-dynamics study
H. Gades and H.M. Urbassek 261
Temporal aspects of sputtering of TaC targets
R.G. Vichev and W. Eckstein 272
An instantaneous inelastic energy loss algorithm for use in molecular dynamics simulations
M.H. Shapiro and T.A. Tombrello 277
Molecular Dynamics studies of cluster emission in sputtering
G. Betz and W. Husinsky 281
Low energy ion irradiation of H-terminated Si(001): hydrogen sputtering, beam-induced (2×1) reconstruction, and Si epitaxy
M.V.R. Murty and H.A. Atwater 293
Molecular dynamics simulation of amorphous silicon sputtering by Ar^+ ions
J.E. Rubio, L.A. Marqués, M. Jaraíz, L.A. Bailón and J. Barbolla 301

Section V. Cluster–solid interactions

Cluster–solid interaction experiments
W.L. Brown and M. Sosnowski 305
Atomic excitation during the impact of ions and clusters
T.A. Tombrello 312
Collision dynamics between gold clusters and gold thin films
Z.Y. Pan and M. Hou 317
Simulation of heavy-ion cluster impact fusion
Y. Yamamura and T. Muramoto 322

Author index 327